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## INFORMATION DISCLOSURE STATEMENT BY APPLICANT

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Sheet 1 of U

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Application Number	10/053,253					
Filing Date	November 2, 2001					
First Named Inventor	Sherman, Michael A.					
Art Unit	1644-1631					
Examiner Name	Unassigned Smith					
Attorney Docket Number	020910-000110US					

			U.S. PATENT D	OCUMENTS	
Examiner	Cite No.1	Document Number  Number Kind Code <sup>2</sup> (if known)	Publication Date MM-DD-YYYY	Name of Patentee or Applicant of Cited Document	Pages, Columns, Lines, Where Relevant Passaries or Relevant Figuris Japopar
<u> </u>	AA	US 6,512,997	1/28/2003	Padilla, et al.	9 2 3
1	AB	US 6,253,166	6/26/2001	Whitmore, et al.	2 2
	AC	US 6,185,506	2/6/2001	Cramer, III, et al.	
	AD	US 6,161,080	12/12/2000	Aouni-Ateshian, et al.	4 6
	AE	US 6,150,179	11/21/2000	Went	# 7
	AF	US 6,125,235	9/26/2000	Padilla, et al.	
	AG	US 6,081,766	6/27/2000	Chapman, et al.	1600129C
	AH	US 6,014,449	171172000	Jacobs, et al.	
	Al .	US 5,799,312	8/25/1998	Rigoutsos	9
	AJ	US 5,787,279	7/28/1998	Rigoutsos	3
	AK	US 5,777,889	7/7/1998	Mohanty, et al	
	AL	US 5,752,019	3/12/1998	Rigoutsos, et al.	
	AM	US 5,745,385	4/28/1998	Hinsberg, III, et al.	
	AN	US 5,625,575	4/29/1997	Goyal, et al.	
	AO	US 5,553,004	9/3/1996	Gronbech-Jensen, et al.	
1	AP	US 5,307,287	4/26/1994	Cramer, III, et al.	

	FOREIGN PATENT DOCUMENTS										
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		Number <sup>4</sup> Country Code <sup>3</sup> (if known)		Publication Date MM-DD-YYYY	Applicant of Cited  Document	Where Relevant Passages or Relevant Figures Appear	1⁵				
C5	AQ	wo	02/073334	A2	07-26-1990	Padilla, et al.					
1	AR	wo	01/67310	Al	12-12-1991	Smith, et al.					
4	AS	wo	96/24902	Al	04-01-1993	Wertz					

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Attorney Docket Number

020910-000110US

ubstitute for form 1449B/PTO Complete if Known **Application Number** 10/053,253 INFORMATION DISCLOSURE Filing Date November 2, 2001 STATEMENT BY APPLICANT **First Named Inventor** Sherman, Michael A. 1644- 1631 Art Unit Smith (use as many sheets as necessary) **Examiner Name** Unassigned-

		OTHER PRIOR ART NON PATENT LITERATURE DOCUMENTS	
Examiner Cite No.1		Include name of the author (in CAPITAL LETTERS), title of the article (when appropriate), title of the item (book, magazine, journal, serial, symposium, catalog, etc.), date, page(s), volume-issue number(s), publisher, city and/or country where published.	ΣΤ <sup>2</sup>
CS	AT	ASCHER, et al., Computer Methods for Ordinary Differential Equations and Differential-Algebraic Equations, 1998, pgs. 3-122 and 231-297, SIAM, Philadelphia, PA.	S
	AU	BARAFF, et al., "Large steps in cloth simulation", 1998, Computer Graphics Proceedings SIGGRAPH 98 (Orlando, July 19-24) p43.pdf.	Alo
	AV	BARTH, et al., "A separating framework for increasing the timestep in molecular dynamics" in Computer Simulation of Biomolecular Systems - Theoretical and Experimental Applications, Volume 3, 1997, pgs. 97-121, Kluwer AcademicDordrecht, The Netherlands.	GENTER 100015
	AW	BERENDSEN, "Molecular Dynamics Simulations: The Limits and Beyond" in Computational Molecular Dynamics: Challenges, Methods, Ideas, 1999, pgs. 3-36, Springer-Verlang, Germany.	
	AX	BISCHOF, et al., <u>ADIFOR 2.0 Users' Guide</u> , 1998, Argonne National Laboratory, University of Chicago, Argonne, IL.	
	AY	BRENAN, et al., <u>Numerical Solution of Initial-Value Problems in Differential-Algebraic Equations</u> , 1989, Chapter 5 (pgs. 115-148), Elsevier Science Publishing Co., New York, NY.	
	AZ	BUTCHER, "Towards efficient implementation of singly-implicit methods", 1988, AMC Transactions of Mathematical Software 14:68-75.	
	ВА	BYSTROFF, "An alternative derivation of the equations of motion in torsion space for a branched linear chain", 2001, Protein Engineering 14:825-828.	
	ВВ	COLEMAN, et al., "The efficient computation of sparse Jacobian matrices using automatic differentiation", 1996, Cornell Theory Center Technical Report CTC95TR225.	
	вс	EICHBERGER, et al., "The benefits of parallel multibody simulation", 1994, International Journal for Numerical Methods in Engineering, 37:1557-1572.	
	BD	GOLUB, et al., "The Differentiation of Pseudo-Inverses and Non-Linear Least Squares Problems Whose Variables Separate", 1973, SIAM J. Numer Anal. 10:413.	
	BE	HAIRER, et al., Solving Ordinary Differential Equations II; Stiff and Differential-Algebraic Problems, 2nd ed., 1996, Springer-Verlang, Germany.	
	BF	HE, et al., "Macromolecular conformational dynamics in torsional angle space", 1998, Journal of Chemical Physics 108:271.	
4	BG	HOLLARS, et al., SD/FAST User's Manual, Version B.2, 1994, Symbolic Dynamics, California.	

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Sheet 3 of

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Application Number	10/053,253					
Filing Date	November 2, 2001					
First Named Inventor	Sherman, Michael A.					
Art Unit	1644- 1631					
Examiner Name	Unassigned Smith					
Attorney Docket Number	020910-000110US	J				

		OTHER PRIOR ART NON PATENT LITERATURE DOCUMENTS				
Examiner Initials *	Cite No.1	Include name of the author (in CAPITAL LETTERS), title of the article (when appropriate), title of the item (book, magazine, journal, serial, symposium, catalog, etc.), date, page(s), volume-issue number(s), publisher, city and/or country where published.	FCH CENTER			
CS	ВН	BH IZAGUIRRE, et al., "Longer Time Steps for Molecular Dynamics", 1999, <u>J.Chem.Phys</u> . 110:9853.				
	Bì	KANE, <u>Dynamics</u> , 3rd ed., 1978, Stanford University, Stanford, California.				
	ВЛ	LEACH, Molecular Modelling Principles and Applications, 2nd ed., 1996, Chapter 6 (pgs. 303-352) Pearson Education Limited, England.				
	ВК	MARTINS, et al., "An automated method for sensitivity analysis using complex variables", 2000, American Institute of Arenautics and Astronoautics, 2000-0689 pl.				
	BL	MOROKUMA, et al., "Model studies of the structures, reactivities, and reaction mechanisms of metalloenzymes", 2001, IBM J. Res. & Dev. 45(3/4):367-395.				
	ВМ	NORSETT, et al., "Embedded SDIRK-methods of basic order three", 1984, BIT 24:634-646.				
	BN	PONDER, TINKER User's Guide, Version 3.8, October 2000, Washington University, St. Louis, MO.				
	ВО	RAPAPORT, The Art of Molecular Dynamics Simulation, 1995, reprinted with corrections 1998, Chapter 3 (pgs. 42-77), Cambridge University Press, United Kingdom.				
	BP	SCHLICK, "Biomolecular Dynamics at Long Timesteps: Bridging the Timescale Gap Between Simulation and Experimentation", 1997, Annu. Rev. Biophys. Biomol. Struct., 26:181-222.				
	BQ	SCHLICK, "Some Failures and Successes of Long-Timestep Approaches to Biomolecular Simulations" in Computational Molecular Dynamics: Challenges, Methods, Ideas, 1999, pgs. 227-262, Springer-Verlang, Germany.				
	BR	SCHLICK, Molecular Modeling and Simulation - An Interdisciplinary Guide, 2002, Chapter 13 and References, pgs. 419-462 and 561-619, Springer-Verlang, Germany.				
	BS	SHAMPINE, "Implementation of implicit formulas for the solution of ODEs", 1980, SIAM J. Sci. Stat. Comput. 1:103-118.				
	вт	VERLET, "Computer Experiments on Classical Fluids. I. Thermodynamical Properties of Lennard-Jones Molecules", 1967, Physical Review, 159(1):98-103.				
V	BU	VON SCHWERIN, Multibody System Simulation, 1999, Springer-Verlang, Germany.				

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Examiner Signature—	(	/ 	andy	51	 Date Considered	2,	19/	04	

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Applicati n Number	10/053,253	
Filing Date	November 2, 2001	
First Named Inventor	Sherman, Michael A.	
Art Unit	1644 - 1631	
Examiner Name	Unassigned Smith	
Attorney Docket Number	020910-000110US	

OTHER PRIOR ART - NON PATENT LITERATURE DOCUMENTS									
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CS	BV	WU, et al., "Constraint dynamics algorithm for simulation of semiflexible macromolecules", 1998, Journal of Computational Chemistry 19:1555-1566							
CS	вw	YEN, et al., "On the numerical solution of constrained multibody dynamic systems", 1994, University of Minnesota AHPCRC 94-038.							

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Examiner Signature	/ 	andy 82	Date Considered	2/9/04

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## INFORMATION DISCLOSURE STATEMENT BY APPLICANT

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Complete if Known				
Application Number	10/053,253			
Filing Date	November 2, 2001			
First Named Inventor	Sherman, Michael A.			
Art Unit	1631			
Examiner Name	Unassigned			
Attorney Docket Number	020910-000110US			

		OTHER PRIOR ART NON PATENT LITERATURE DOCUMENTS				
Examiner Cite Initials * No.1		Include name of the author (in CAPITAL LETTERS), title of the article (when appropriate), title of the item (book, magazine, journal, serial, symposium, catalog, etc.), date, page(s), volume-issue number(s), publisher, city and/or country where published.				
CS		ABAGYAN, et al., "New Methodology for Computer-Aided Modelling of Biomolecular Structure and Dynamics 2. Local Deformation Cycles", 1989, Journal of Biomolecular Structure & Dynamics 6(4):833-845.				
		GIBSON, et al., "Variable Step Molecular Dynamics: An Exploratory Technique for Peptides with Fixed Geometry", 1990, Journal of Computational Chemistry 11(4):468-486.				
		JAIN, et al., "Linearization of Manipulator Dynamics Using Spatial Operators", 1993, IEEE Transactions on Systems, Man and Cybernetics 23(1):239-248.				
		LUDOVICE, et al., "Molecular dynamics of geometrically constrained polymer systems in generalized coordinates: Basic formalism", 1991, Computational Polymer Science 1:69-79.				
		MAZUR, et al., "New Methodology for Computer-Aided Modelling of Biomolecular Structure and Dynamics 1. Non-Cyclic Structures", 1989, Journal of Biomolecular Structure & Dynamics 6(4):815-832.				
		PESKIN, ET AL., "Molecular Dynamics by the Backward-Euler Method", 1989, Communications on Pure and Applied Mathematics XLII:1011-1031.				
		ROSENTHAL, et al., "High Performance Multibody Simulations via Symbolic Equation Manipulation and Kane's Method", 1986, The Journal of the Astronautical Sciences, 34(3):223-239.				
		ROSENTHAL, "An Order n Formulation for Robotic Systems", 1990, The Journal of the Astronautical Sciences, 38(4):511-529.				
	-	ROSENTHAL, "Engineers Notes: Triangulation of Equations of Motion for Robotic Systems", 1988, The Journal of Guidance, 11(3):278-281.				
		SCHLICK, et al., "A molecular dynamics simulation of a water droplet by the implicit Euler/Langevin scheme", 1991, J. Chem. Phys., 94(3):2118-2129.				
1		ZHANG, et al., "The Langevin/implicit-Euler/normal-mode scheme for molecular dynamics at large timesteps", 1994, J. Chem. Phys. 101(6):4995-5012.				

Examiner Signature	andy or	Date Considered	5/5/04

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November 2, 2000

Sherman, Michael A

Unassigned Smith

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STATEMENT BY APPLICANT

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,11'' <u>-</u>	U.S. PATENT DOCUMENTS						
Examiner Initials *	Cite No.	U.S. Patent Document  Number Kind Code <sup>2</sup> (if known)	Name of Patentee or Applicant of Cited Document	Date of Publication of Cited Document MM-DD-YYYY	Pages, Columns, Lines, Where Relevant Passages or Relevant Figures Appear	-8	
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**Application Number** 

First Named Inventor

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<sup>1</sup> Unique citation designation number. 2 See attached Kinds of U.S. Patent Documents. 3 Enter Office that issued the document, by the two-letter code (WIPO Standard ST.3). 4 For Japanese patent documents, the indication of the year of the reign of the Emperor must precede the serial number of the patent document. 5 Kind of document by the appropriate symbols as indicated on the document under WIPO Standard ST. 16 if possible. 6 Applicant is to place a check mark here if English language Translation is attached.

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Application Number	10/053,253	
Filing Dat	November 2, 2000	31
First Named Invent r.	Sherman, Michael A.	우
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	OTHER PRIOR ART - NON PATENT LITERATURE DOCUMENTS					
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CS	AC	LEUNG et al., "Concurrent DASSL: A Second-Generation DAE Solver Library," IEEE Proceedings of Scalable Libraries Conference, from conference held 10/6-8/93 at Syracuse University, New York, NY, pgs. 204-210.				
CS	AD	ABDEL-RAHMAN et al., "Determination of the Ligamentous and Contact Forces in the Human Tibio – Femoral Joint Using a Three – Dimensional Dynamic Anatomical Model," <u>IEEE Proceedings of Biomedical Engineering Conference</u> , from conference held 3/29-31/96 in Dayton Ohio, pgs. 373-376.				
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